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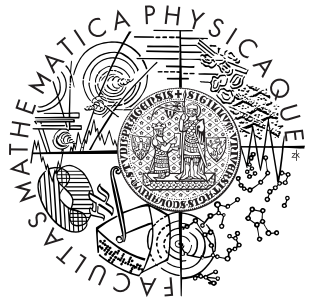

Daniel Božík

Teorie založené na energetických funkcionálech v jaderné fyzice

Ústav částicové a jaderné fyziky, MFF UK

Vedoucí bakalářské práce: prof. RNDr. Jan Kvasil, DrSc.,
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Chcel by som poďakovať prof. RNDr. Janovi Kvasilovi, DrSc. za pomoc pri štúdiu teórie a mnohé užitočné rady a pripomienky pri písaní práce. Takisto by som za pomoc pri štúdiu teórie chcel poďakovať aj Mgr. Petrovi Veselému, rovnako ako aj za pomoc pri práci s použitými počítačovými programami.

Prohlašuji, že jsem svou bakalářskou práci napsal samostatně a výhradně s použitím citovaných pramenů. Souhlasím se zapůjčováním práce a jejím zveřejňováním.

V Praze dne 1.8.2008 Daniel Božík

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Vedoucí bakalářské práce: prof. RNDr. Jan Kvasil, DrSc.
e-mail vedoucího: kvasil@ipnp.troja.mff.cuni.cz

Abstrakt: Obsahom tejto práce je skúmanie elektromagnetických prechodov E1 a E2 v sférickom jadre ^{92}Mo a deformovanom jadre ^{102}Mo. Teoreticky je tento problém riešený použitím štyroch parametrizácií Skyrme interakcie - `SkM*, SkT6, SLy6, SkI3`. Zo Skyrme hamiltoniánu vyjadreného vo forme energetického funkcionálu sa riešením Hartree-Fock-Bogoljubovových rovníc získa self-konzistentné stredné pole. Zvyšková interakcia sa separabilizuje - separabilnou formou RPA metódy potom získavame prechodové excitačné spektrá daných multipolarít. Problém je riešený použitím série počítačových programov vyvinutých na University in Erlangen, JINR Dubna v Rusku a v Ústave částicové a jaderné fyziky na Karlové univerzite, ktoré implementujú tieto metódy. Na konci práce je diskusia výsledkov a porovnanie výsledkov so započítaním zvyškovej interakcie a bez nej.
Klíčová slova: Skyrme interakcia, energetický funkcionál, separabilná RPA metóda, elektromagnetické prechody, HFB metóda

Title: Energy functional theories in nuclear physics
Author: Daniel Božík
Department: Institute of Particle and Nuclear Physics of Charles University
Supervisor: prof. RNDr. Jan Kvasil, DrSc.
Supervisor's e-mail address: kvasil@ipnp.troja.mff.cuni.cz

Abstract: Abstract: In this bachelor thesis we investigate the electromagnetic transitions of the E1 and E2 type in the spherical nucleus ^{92}Mo and the deformed nucleus ^{102}Mo. Theoretically this problem is solved using four parametrizations of the effective Skyrme interaction - `SkM*, SkT6, SLy6, SkI3`. By solving the Hartree-Fock-Bogoliubov equations for the functional form of the Skyrme Hamiltonian we gain the self-consistent mean-field. The residual interaction is factorized into the separable form - then using the separable-RPA method we get the transition excitation spectra of given multipolarities. The actual solution of the problem was provided by the chain of numerical codes - created on the University in Erlangen, the JINR Dubna

in Russia and the Institute of Particle and Nuclear Physics of Charles University - which implement these theoretical methods. In the last part of the thesis we discuss the results and also compare them for the case with or without including the residual interaction.
Keywords: Skyrme interaction, energy functional, separable RPA method, electromagnetic transitions, HFB method

1 Introduction

Skyrme interaction as an effective nuclear force has been established, in the last two decades, for Hartree-Fock (HF) and Hartree-Fock-Bogoliubov (HFB) calculations. Originally introduced in the paper of T.H.R. Skyrme [9], Skyrme interaction consists of two-body and three-body part

$$V_{Sk} = \sum_{i<j} \mathcal{V}_{ij}^{(2)}(Sk) + \sum_{i<j<k} \mathcal{V}_{ijk}^{(3)}(Sk). \tag{1.1}$$

Since very simple phenomenological formula for the three-body part of the force

$$\mathcal{V}_{Sk}^{(3)}(\vec{r}_i, \vec{r}_j, \vec{r}_k) = t_3 \delta(\vec{r}_i - \vec{r}_j)\delta(\vec{r}_j - \vec{r}_k) \tag{1.2}$$

it is possible, within the even-even spin-saturated nuclei, to replace the three-body part by the density-dependent two-body operator

$$\mathcal{V}_{Sk,dens.}^{(2)}(\vec{r}_i, \vec{r}_j) = \frac{1}{6} t_3 (1 + \kappa_3 \hat{P}_\sigma)\delta(\vec{r}_i - \vec{r}_j)\rho^\alpha \left(\frac{\vec{r}_i + \vec{r}_j}{2} \right). \tag{1.3}$$

Such form of a density-dependent (two-body) effective Skyrme force, appearing in the 70^{th} for instance in the paper [11], became the standard prescription for all presently used Skyrme parametrizations.

Once introduced, this density-dependent effective nuclear force is employed in the selfconsistent Hartree-Fock (or Hartree-Fock-Bogoliubov) method to build up nuclear Hamiltonian as a sum of single-(quasi)particle mean-field $\hat{h}_{HFB}$ and the corresponding residual interaction $\hat{V}_{res}$

$$\hat{H} = \hat{h}_{HFB} + \hat{V}_{res}. \tag{1.4}$$

Since usually there is used an approximation that the global properties of nucleus (the bulk properties) as for example binding energy, nuclear radii or compressibility of the nuclear matter are determined by the mean-field part of the nuclear Hamiltonian $\hat{h}_{HFB}$, all the reasonable Skyrme parametrizations were tuned by fitting the bulk properties of several chosen nuclei to the experimental values.

In order to describe more detailed nuclear properties (excited states, electromagnetic transitions and giant resonances), it is necessary to take into account residual interaction $\hat{V}_{res}$. This is usually done in the framework of the Random Phase Approximation (RPA) which is nothing more than

the limit of small-amplitude harmonic vibrations around the ground state. However, since the solution of the full RPA equations (especially in the case of deformed systems) is time consuming, for the purposes of systematic studies of the heavier and heavy elements, there was developed a separable form of RPA (see e.g. [6]).

The main task of this bachelor thesis is to acquaint with the chain of codes built up for the description of transition spectra in heavier spherical, as well as deformed nuclei. These codes solve the self-consistent HFB problem with effective Skyrme interaction and then factorize the full Skyrme residual interaction into the separable form, according to the recipe given in [6] and solve the separable RPA equation. As a result these codes find the RPA states - energies and two-quasiparticle amplitudes. These codes also determine the excitation strength functions (energy distribution functions of the excitation probability) of different types (electric and magnetic) and different multipolarities (dipole, quadrupole, ...). In this bachelor thesis the codes mentioned above are used for the determination of the isovector electric dipole strength function (isovector dipole giant resonance - (IVGDR) and isoscalar giant quadrupole resonance - (ISGQR)) in two Mo isotopes: spherical ^{92}Mo and deformed ^{102}Mo. In the thesis we discuss differences between spherical and deformed cases.
The thesis is organized in the following way. In the Chapter 2 is given a brief description of the theoretical approach. The Chapter 3 is devoted to the discussion of obtained results and in the Chapter 4 are presented some concluding remarks.

2 Theoretical outline

The effective density dependent Skyrme interaction – as briefly mentioned in the previous chapter – has the following form

$$V_{Sk} = \sum_{i<j} \mathcal{V}_{ij}^{(2)}(Sk) + \sum_{i<j} \mathcal{V}_{ij}^{(2)}(Sk, dens.) \tag{2.1}$$

where in the coordinate-spin representation (see e.g. [8])

$$\begin{aligned} \mathcal{V}_{Sk}^{(2)}(\vec{r}_i\vec{\sigma}_i, \vec{r}_j\vec{\sigma}_j) &= t_0(1+\kappa_0\hat{P}_\sigma)\delta(\vec{r}_i-\vec{r}_j) + \\ &+ \frac{t_1}{2}(1+\kappa_1\hat{P}_\sigma)[\delta(\vec{r}_i-\vec{r}_j)\vec{k}^2 + \overleftarrow{k}^{\,2}\delta(\vec{r}_i-\vec{r}_j)] + \\ &+ t_2(1+\kappa_2\hat{P}_\sigma)\overleftarrow{k}\,\delta(\vec{r}_i-\vec{r}_j)\vec{k} + \mathrm{i}V_{S.O.}(\vec{\sigma}_i+\vec{\sigma}_j)\cdot\overleftarrow{k}\times\delta(\vec{r}_i-\vec{r}_j)\vec{k} \end{aligned} \tag{2.2}$$

and

$$\mathcal{V}_{Sk,dens.}^{(2)}(\vec{r}_i, \vec{r}_j, \vec{r}_k) = \frac{1}{6}t_3(1+\kappa_3\hat{P}_\sigma)\delta(\vec{r}_i-\vec{r}_j)\rho^\alpha\left(\frac{\vec{r}_i+\vec{r}_j}{2}\right) \tag{2.3}$$

where $\vec{k} = \frac{\vec{\nabla}_i - \vec{\nabla}_j}{2\mathrm{i}}$ acts on the right direction and $\overleftarrow{k} = -\frac{\overleftarrow{\nabla}_i - \overleftarrow{\nabla}_j}{2\mathrm{i}}$ acts on the left direction. In order to gain the total effective nucleon-nucleon interaction we add the Coulomb interaction between protons (in the coordinate representation)

$$\mathcal{V}_{Coul}^{(2)}(\vec{r}_i, \vec{r}_j) = \frac{e^2}{4\pi\varepsilon_0(\vec{r}_i-\vec{r}_j)} \tag{2.4}$$

and the short-range pairing interaction (expressed in the representation of creation and annihilation operators $a_i^\dagger$, a_i)

$$\hat{V}_{pair} = \sum_{\tau=n,p} G_\tau \left(\sum_i a_i^\dagger a_{\overline{i}}^\dagger\right)\left(\sum_j a_{\overline{j}} a_j\right) \tag{2.5}$$

to the Skyrme interaction (2.1).
In the eqs. (2.2), (2.3), (2.5) we introduced the interaction strength constants t_0, t_1, t_2, t_3, κ_0, κ_1, κ_2, κ_3, $V_{S.O.}$, G_τ and also $\hat{P}_\sigma$ which is the spin exchange operator in the spin part of the configuration space.
In order to use HF (or HFB) method to obtain single-particle (or single-quasiparticle) mean field $\hat{h}_{HF}$ (or $\hat{h}_{HFB}$), we need the expectation value of

the nuclear Hamiltonian (1.4) in the trial Slater determinants (or quasiparticle vacua) $|\Psi\rangle$, which gives us the so called energy functional, $\langle\Psi|\hat{H}|\Psi\rangle$, of trial single-particle wave functions (or densities and currents). For the Skyrme interactions (2.1), (2.2), (2.3), with the pairing interaction (2.5) this energy functional has the following form

$$\mathcal{E} = \langle\Psi|\hat{H}|\Psi\rangle = \int \mathrm{d}^3r \left(\mathcal{H}_{kin}(\vec{r}) + \mathcal{H}_{Skyr}(\vec{r}) + \mathcal{H}_{Coul}(\vec{r}) + \mathcal{H}_{pair}(\vec{r})\right) \quad (2.6)$$

where

$$\mathcal{H}_{kin}(\vec{r}) = \frac{\hbar^2}{2m}\tau(\vec{r}) \quad (2.7a)$$

$$\mathcal{H}_{Coul}(\vec{r}) = \frac{e^2}{4\pi\varepsilon_0 c}\int \mathrm{d}^3r'\,\rho_p(\vec{r}') - \frac{3}{4}\frac{e^2}{4\pi\varepsilon_0 c}\left(\frac{3}{4}\right)^{1/3}(\rho_p(\vec{r}))^{4/3} \quad (2.7b)$$

$$\begin{aligned}
\mathcal{H}_{Skyr}(\vec{r}) = {} & \frac{b_0}{2}\rho^2 - \frac{b_0'}{2}\sum_{\tau=n,p}\rho_\tau^2 - \frac{b_2}{2}\rho(\Delta\rho) + \frac{b_2'}{2}\sum_{\tau=n,p}\rho_\tau(\Delta\rho_\tau) + \\
& + \frac{b_3}{3}\rho^{\alpha+2} - \frac{b_3'}{3}\rho^\alpha\sum_{\tau=n,p}\rho_\tau^2 + b_1(\rho\tau - \vec{j}^2) - b_1'\sum_\tau\left(\rho_\tau\tau_\tau - \vec{j}_\tau^2\right) - \\
& - b_4[\rho(\vec{\nabla}\cdot\vec{J}) + \vec{s}\cdot(\vec{\nabla}\times\vec{j})] - b_4'\sum_{\tau=n,p}\left[\rho_\tau\left(\vec{\nabla}\cdot\vec{J}\right)_\tau + \vec{s}_\tau\cdot(\vec{\nabla}\times\vec{j}_\tau)\right] + \\
& + \widetilde{b}_4[\vec{s}\cdot\vec{T} - \vec{J}^2] + \widetilde{b}_4'\sum_{\tau=n,p}\left(\vec{s}_\tau\cdot\vec{T}_\tau - \vec{J}_\tau^2\right) + \\
& + b_5\rho(\rho\tau - \vec{j}^2) - b_5'\rho\sum_{\tau=n,p}(\rho_\tau\tau_\tau - \vec{j}_\tau^2) - \\
& - \frac{b_6}{2}\rho^2(\Delta\rho) + \frac{b_6'}{2}\rho\sum_{\tau=n,p}\rho_\tau(\Delta\rho_\tau) + \\
& + \widetilde{b}_5\vec{s}^2 + \widetilde{b}_5'\sum_{\tau=n,p}\vec{s}_\tau^2 + \widetilde{b}_6\rho^\xi\vec{s}^2 - \widetilde{b}_6'\rho^\xi\sum_{\tau=n,p}\vec{s}_\tau^2 + \\
& + \widetilde{b}_7\vec{s}(\Delta\vec{s}) + \widetilde{b}_7'\sum_{\tau=n,p}\vec{s}_\tau(\Delta\vec{s}_\tau) + \widetilde{b}_8(\vec{\nabla}\vec{s})^2 + \widetilde{b}_8'\sum_{\tau=n,p}(\vec{\nabla}\vec{s}_\tau)^2
\end{aligned} \quad (2.7c)$$

and

$$\mathcal{H}_{pair}(\vec{r}) = \frac{1}{4}\sum_{\tau=n,p}\chi_\tau^2(\vec{r})G_\tau \quad (2.7d)$$

In (2.7) b_0, b_0', b_2, b_2', b_3, b_3', b_1, b_1', b_4, b_4', $\widetilde{b}_4$, $\widetilde{b}_4'$, b_5, b_5', b_6, b_6', $\widetilde{b}_5$, $\widetilde{b}_5'$, $\widetilde{b}_6$, $\widetilde{b}_6'$, $\widetilde{b}_7$, $\widetilde{b}_7'$, $\widetilde{b}_8$, $\widetilde{b}_8'$, $V_\tau^{(0)}$, α, ξ are constants directly related tho the strength

constants t_0, t_1, t_2, t_3, κ_0, κ_1, κ_2, κ_3, $V_{S.O.}$, G_τ in (2.2), (2.3), (2.5) (see e.g. [8, 10]).
Quantities $J_\tau^{(\alpha)}(\vec{r}) \equiv \rho_\tau(\vec{r})$, $\tau_\tau(\vec{r})$, $\vec{J}_\tau(\vec{r})$, $\vec{j}_\tau(\vec{r})$, $\vec{s}_\tau(\vec{r})$, $\vec{T}_\tau(\vec{r})$, $\chi_\tau(\vec{r})$ ($\tau = n, p$; $J^{(\alpha)}(\vec{r}) = \vec{J}_n(\vec{r}) + \vec{J}_p(\vec{r})$) are densities and currents:

$$J^{(\alpha)}(\vec{r}) \equiv \langle\Psi|\hat{J}^{(\alpha)}(\vec{r})|\Psi\rangle \qquad\qquad \alpha = \rho,\, \tau,\, \vec{y},\, \vec{j},\, \vec{s},\, \vec{T},\, \chi \tag{2.8}$$

where $\hat{J}^{(\alpha)}(\vec{r})$ are density and current operators:

$$\begin{aligned}
\hat{\rho}(\vec{r}) &= \sum_\tau \sum_{i,j\in\tau} \psi_i^\dagger(\vec{r})\psi_j(\vec{r})\, a_i^\dagger a_j \\
\hat{\tau}(\vec{r}) &= \sum_\tau \sum_{i,j\in\tau} (\vec{\nabla}\psi_i(\vec{r}))^\dagger(\vec{\nabla}\psi_j(\vec{r}))\, a_i^\dagger a_j \\
\vec{y}(\vec{r}) &= -\frac{\mathrm{i}}{2} \sum_\tau \sum_{i,j\in\tau} \{\psi_i^\dagger(\vec{r})(\vec{\nabla}\times\psi_j(\vec{r})) + (\vec{\nabla}\times\psi_i(\vec{r}))^\dagger\psi_j(\vec{r})\}\, a_i^\dagger a_j \\
\vec{j}(\vec{r}) &= \frac{\mathrm{i}}{2} \sum_\tau \sum_{i,j\in\tau} \{\vec{\nabla}\psi_i(\vec{r}))^\dagger\psi_j(\vec{r}) - \psi_i^\dagger(\vec{r})(\vec{\nabla}\psi_j(\vec{r}))\}\, a_i^\dagger a_j \\
\hat{\vec{s}}(\vec{r}) &= \sum_\tau \sum_{i,j\in\tau} \psi_i^\dagger(\vec{r})\vec{\sigma}\psi_j(\vec{r})\, a_i^\dagger a_j \\
\hat{\vec{T}}(\vec{r}) &= \sum_\tau \sum_{i,j\in\tau} (\vec{\nabla}\psi_i(\vec{r}))^\dagger\vec{\sigma}(\vec{\nabla}\psi_j(\vec{r}))\, a_i^\dagger a_j \\
\hat{\chi}_\tau(\vec{r}) &= \sum_{i\in\tau} \psi_i^\dagger(\vec{r})\psi_i(\vec{r})(a_i^\dagger a_{\bar{\tau}}^\dagger + a_{\bar{\imath}} a_i)
\end{aligned} \tag{2.9}$$

where $\psi_i(\vec{r}) = \begin{pmatrix}\varphi_i(\vec{r},\uparrow)\\ \varphi_i(\vec{r},\downarrow)\end{pmatrix}$ are the trial single particle spinor functions. HF variational principle (variations with respect to the trial functions $\psi_i(\vec{r})$):

$$\delta\left\{\mathcal{E} - e_i \int \mathrm{d}^3r\, \psi_i^\dagger(\vec{r})\psi_i(\vec{r})\right\} = 0 \tag{2.10}$$

gives the equilibrium Slater determinant $|\Psi\rangle_0$, equilibrium single-particle spinors $\psi_i^{(0)}(\vec{r})$ with corresponding single-particle energies e_i and similarly also the single-quasiparticle HF field $\hat{h}_{HF}$ ($\hat{h}_{HF}|i\rangle = e_i|i\rangle$):

$$\hat{h}_{HF} = \int \hat{h}_{HF}(\vec{r})\, \mathrm{d}^3r \qquad \hat{h}_{HF}(\vec{r}) = \sum_{\substack{\tau\alpha \\ \alpha=\rho,\tau,\vec{y},\vec{j},\vec{s},\vec{T}}} \frac{\partial\mathcal{E}}{\partial J_\tau^{(\alpha)}(\vec{r})} \hat{J}_\tau^{(\alpha)}(\vec{r}) \tag{2.11}$$

Subsequently (within each HF iteration) we solve the Bardeen-Cooper-Schiefer (BCS) method and gain thus the HFB mean field Hamiltonian:

$$\hat{h}_{HFB} = \hat{h}_{HF} + \int \sum \tau \frac{\partial \mathcal{E}}{\partial \chi_\tau(\vec{r})} \hat{\chi}_\tau(\vec{r})\, \mathrm{d}^3 r\,. \tag{2.12}$$

In the quasiparticle formalism the HFB mean-field Hamiltonian has the diagonal form (see e.g. [8]):

$$\hat{h}_{HFB} = \langle HFB|\hat{H}|HFB\rangle + \sum_{\substack{\nu \\ \nu>0}} E_\nu(\alpha^\dagger_\nu \alpha_\nu + \alpha^\dagger_{\overline{\nu}} \alpha_{\overline{\nu}}) \tag{2.13}$$

where quasiparticle creation ($\alpha^\dagger_\nu$) and annihilation (α_ν) operators are given by Bogoliubov transformation

$$\begin{aligned} a^\dagger_\nu &= \mathcal{U}_\nu \alpha^\dagger_\nu + \mathcal{V}_\nu \alpha_{\overline{\nu}} \\ a^\dagger_{\overline{\nu}} &= \mathcal{U}_\nu \alpha^\dagger_{\overline{\nu}} - \mathcal{V}_\nu \alpha_\nu, \qquad \alpha_\nu|HFB\rangle = 0 \end{aligned} \tag{2.14}$$

with

$$\mathcal{U}^2_\nu = \frac{1}{2}\left\{1 + \frac{e_\nu - \lambda_\tau}{\sqrt{(e_\nu - \lambda_\tau)^2 + \Delta^2_\tau}}\right\} \quad \mathcal{V}^2_\nu = \frac{1}{2}\left\{1 - \frac{e_\nu - \lambda_\tau}{\sqrt{(e_\nu - \lambda_\tau)^2 + \Delta^2_\tau}}\right\} \tag{2.15}$$

$$E_\nu = \sqrt{(e_\nu - \lambda_\tau)^2 + \Delta^2_\tau} \tag{2.16}$$

where λ_τ ($\tau = n, p$) are the neutron and proton Fermi energies, and $\Delta_\tau = -G_\tau \sum_\nu \mathcal{U}_\nu \mathcal{V}_\nu$ are the neutron and proton pairing gap energies, E_ν are single-quasiparticle energies.

In the next step, in order to describe also collective excitations of our system (nucleons), we should take into account residual interaction $\hat{V}_{res} = \hat{H} - \hat{h}_{HF}$. As it was mentioned in the Chapter 1 – for the systematic study of the heavy deformed nuclei it is worth to factorize the full residual interaction to the separable form. Therefore, instead of using usual (full) RPA method we used a multidimensional linear response theory introduced in [5, 7], which is equivalent to the RPA with special separable interaction (separable RPA – SRPA). The brief description of the multidimensional linear response theory is the following.

The starting ansatz is that the system (nucleus) is excited by a set of Hermitian single particle operators $(\hat{Q}_k,\, \hat{P}_k)$ $(k = 1, \ldots, N)$ where

$$\begin{aligned} &\hat{Q}_k^\dagger = \hat{Q}_k \qquad && \hat{T}^{-1}\hat{Q}_k\hat{T} = \hat{Q} \qquad && \hat{P}_k^\dagger = \hat{P}_k \\ &\hat{P}_k = i\left[\hat{H}, \hat{Q}_k\right] \qquad && \hat{T}^{-1}\hat{P}_k\hat{T} = -\hat{P} \qquad && \hat{Q}_k = i\left[\hat{H}, \hat{P}_k\right] \end{aligned} \tag{2.17}$$

where $\hat{T}$ is the time-reverse transformation. As a result of the action of these exciting operators $(\hat{Q}_k,\, \hat{P}_k)$, the system (nucleus) vibrates around its ground state $|HFB\rangle$. By the appropriate choice of the exciting modes we can regulate the type and multipolarity of the excitation we want to study. For instance, if we intend to study quadrupole electric $E2$ excitations, we excite the nucleus by operators $(\hat{Q}_k,\, \hat{P}_k)$, where $\hat{Q}_k$ is the quadrupole operator ($\hat{Q}_k = \sum_{i,j}\left(\int \mathrm{d}^3 r\, \varphi_i(\vec{r},\sigma_i) f(r) Y_{2\mu}(\vec{r}) \varphi_j(\vec{r},\sigma_j)\right) a_i^\dagger a_j$) with different radial dependence $f(r)$ (e.g. $f(r) = r^2, r^4, j_2(qr), \ldots$).
The choice of the radial dependence influences how deeply we want to excite the nucleus. It can be shown (see e.g. [5]) that if we take only quadrupole operator with $f(r) = r^2$, corresponding excitations involve only configurations situated on the nucleus surface. Involving higher power radial dependence (r^{2+p} with $p > 0$ or $j_2(qr)$) causes that more deep configurations inside the nucleus participate in the building up investigated quadrupole excitations. One operator (with $p = 0$) or two operators (with $p = 0, 1$) are usually sufficient for the description of excitations of given multipolarity.
Vibrations of the nucleus, caused by the external modes (2.17), are described by the time-dependent HFB vacuum $|HFB(t)\rangle$ which is related to the equilibrium HFB vacuum $|HFB\rangle$ (see (2.14)) by the time-dependent shift transformation (see e.g. [4]):

$$|HFB(t)\rangle = \prod_{\tau=n,p}\prod_{k=1}^{N} \mathrm{e}^{-\mathrm{i}(q_{k\tau}(t)-\langle q_{k\tau}\rangle)\hat{Q}_{k\tau}} \mathrm{e}^{-\mathrm{i}p_{k\tau}(t)\hat{P}_{\tau k}} |HFB\rangle \tag{2.18}$$

where $q_{k\tau}(t) - \langle q_{k\tau}\rangle$ and $p_{k\tau}(t)$ are periodical vibration amplitudes

$$\begin{aligned} q_{k\tau}(t) - \langle q_{k\tau}\rangle &= \langle HFB(t)|\hat{Q}_{k\tau}|HFB(t)\rangle - \langle HFB|\hat{Q}_{k\tau}|HFB\rangle = \\ &= \overline{q}_{k\tau}\cos\omega t \\ p_{k\tau}(t) &= \langle HFB(t)|\hat{P}_{k\tau}|HFB(t)\rangle = \overline{p}_{k\tau}\sin\omega t \end{aligned} \tag{2.19}$$

Using the Taylor decomposition of (2.18) up to the linear order in amplitudes $q_{k\tau}(t) - \langle q_{k\tau}\rangle$, $p_{k\tau}(t)$, we obtain for time-dependent densities and currents

$J^{(\alpha)}_\tau(\vec{r},t)$ (see (2.8), (2.9)) the following expressions

$$\begin{aligned} J^{(\alpha)}_\tau(\vec{r},t) &= \langle HFB|\hat{J}^\alpha(\vec{r})|HFB\rangle + \delta J^{(\alpha)}_\tau(\vec{r},t) = \\ &= J^{(\alpha)}_\tau(\vec{r}) + \delta J^{(\alpha)}_\tau(\vec{r},t) \end{aligned} \tag{2.20}$$

with

$$\begin{aligned} \delta J^{(\alpha)}_\tau(\vec{r},t) &= \langle HFB(t)|\hat{J}^{(\alpha)}_\tau(\vec{r})|HFB(t)\rangle - \langle HFB|\hat{J}^{(\alpha)}_\tau(\vec{r})|HFB\rangle \approx \\ &\approx -\mathrm{i}\sum_{\tau k}\Big((q_{k\tau}(t)-\langle q_{k\tau}\rangle)\langle HFB|[\hat{P}_{k\tau},\hat{J}^{(\alpha)}_\tau(\vec{r})]|HFB\rangle + \\ &\quad + p_{k\tau}(t)\langle HFB|[\hat{Q}_{k\tau},\hat{J}^{(\alpha)}_\tau(\vec{r})]|HFB\rangle\Big) \end{aligned} \tag{2.21}$$

Similarly for the time-dependent (vibrating) HFB mean field (see (2.11), (2.12))up to the linear order in $q_{k\tau}(t)-\langle q_{k\tau}\rangle$, $p_{k\tau}(t)$ we have

$$\begin{aligned} \delta\hat{h}_{HFB}(\vec{r},t) &= \sum_{\alpha',\tau'}\frac{\partial\hat{h}_{HFB}(\vec{r})}{\partial J^{(\alpha')}_{\tau'}(\vec{r}')}\delta J^{(\alpha')}_{\tau'}(\vec{r}',t) = \\ &= \int \mathrm{d}^3r'\sum_{\substack{\alpha\tau\\ \alpha'\tau'}}\left[\frac{\partial^2\mathcal{E}}{\partial J^{(\alpha)}_\tau(\vec{r})\partial J^{(\alpha')}_{\tau'}(\vec{r}')}\right]\delta J^{(\alpha')}_{\tau'}(\vec{r}',t)\hat{J}^{(\alpha)}_\tau(\vec{r}) = \\ &= \sum_{\tau k}\Big\{(q_{k\tau}(t)-\langle q_{k\tau}\rangle)\hat{X}_{k\tau}(\vec{r}) + p_{k\tau}(t)\hat{Y}_{k\tau}(\vec{r})\Big\} \\ \delta\hat{H}_{HFB}(t) &= \int \mathrm{d}^3r\,\delta\hat{h}_{HFB}(\vec{r},t) \end{aligned} \tag{2.22}$$

where we introduced following operators

$$\begin{aligned} &\hat{X}_{k\tau}(\vec{r}) = \sum_{\tau'}\hat{X}^{\tau'}_{k\tau}(\vec{r}) = \\ &= \mathrm{i}\int \mathrm{d}^3r'\sum_{\substack{\alpha_+,\alpha'_+\\ \tau'}}\left[\frac{\partial^2\mathcal{E}}{\partial J^{(\alpha_+)}_\tau(\vec{r})\partial J^{(\alpha'_+)}_{\tau'}(\vec{r}')}\right]\langle HFB|\left[\hat{P}_{k\tau'},\hat{J}^{(\alpha'_+)}_{\tau'}(\vec{r}')\right]|HFB\rangle\hat{J}^{(\alpha_+)}_\tau(\vec{r}) \\ &\hat{Y}_{k\tau}(\vec{r}) = \sum_{\tau'}\hat{Y}^{\tau'}_{k\tau}(\vec{r}) = \\ &= \mathrm{i}\int \mathrm{d}^3r'\sum_{\substack{\alpha_-,\alpha'_-\\ \tau'}}\left[\frac{\partial^2\mathcal{E}}{\partial J^{(\alpha_-)}_\tau(\vec{r})\partial J^{(\alpha'_-)}_{\tau'}(\vec{r}')}\right]\langle HFB|\left[\hat{Q}_{k\tau'},\hat{J}^{(\alpha'_-)}_{\tau'}(\vec{r}')\right]|HFB\rangle\hat{J}^{(\alpha_-)}_\tau(\vec{r}) \end{aligned} \tag{2.23}$$

where α_+ enumerates T-even densities ($\hat{T}^{-1}\hat{J}^{(\alpha_+)}\hat{T} = \hat{J}^{(\alpha_+)}$) and α_- enumerates T-odd densities ($\hat{T}^{-1}\hat{J}^{(\alpha_-)}\hat{T} = -\hat{J}^{(\alpha_-)}$). Finally we gain

$$\begin{aligned} \hat{X}_{k\tau} &= \int \mathrm{d}^3 r\, \hat{X}_{k\tau}(\vec{r}) & \hat{T}^{-1}\hat{X}_{k\tau}\hat{T} &= \hat{X}_{k\tau} \\ \hat{Y}_{k\tau} &= \int \mathrm{d}^3 r\, \hat{Y}_{k\tau}(\vec{r}) & \hat{T}^{-1}\hat{Y}_{k\tau}\hat{T} &= -\hat{Y}_{k\tau} \end{aligned} \tag{2.24}$$

For time-dependent variations of operators $\hat{X}_{k\tau}$ and $\hat{Y}_{k\tau}$ we have (similarly as in (2.21) for $\delta J^{(\alpha)}_\tau(\vec{r},t)$)

$$\begin{aligned} \langle \delta\hat{X}_{k\tau}(t)\rangle &= \langle HFB(t)|\hat{X}_{k\tau}|HFB(t)\rangle - \langle HFB|\hat{X}_{k\tau}|HFB\rangle = \\ &= \sum_{k'\tau'} (q_{k'\tau'}(t) - \langle q_{k\tau}\rangle)\kappa^{-1}_{k\tau,k'\tau'} \\ \langle \delta\hat{Y}_{k\tau}(t)\rangle &= \langle HFB(t)|\hat{Y}_{k\tau}|HFB(t)\rangle - \langle HFB|\hat{Y}_{k\tau}|HFB\rangle = \\ &= \sum_{k'\tau'} p_{k'\tau'}(t)\eta^{-1}_{k\tau,k'\tau'} \end{aligned} \tag{2.25}$$

where we introduced strength constants $\kappa^{-1}_{k\tau,k'\tau'}$ and $\eta^{-1}_{k\tau,k'\tau'}$

$$\begin{aligned} &\kappa^{-1}_{k\tau,k'\tau'} = \kappa^{-1}_{k'\tau',k\tau} \equiv \mathrm{i}\langle HFB|\left[\hat{P}_{k'\tau'},\hat{X}_{k\tau}\right]|HFB\rangle = \\ &= \int \mathrm{d}^3 r \int \mathrm{d}^3 r' \sum_{\alpha_+\alpha'_+} \langle HFB|\left[\hat{P}_{k\tau},\hat{J}^{(\alpha_+)}_\tau(\vec{r})\right]|HFB\rangle \left[\frac{\partial^2\mathcal{E}}{\partial J^{(\alpha_+)}_\tau(\vec{r})\partial J^{(\alpha'_+)}_{\tau'}(\vec{r}')}\right] \\ &\quad \langle HFB|\left[\hat{P}_{k'\tau'},\hat{J}^{(\alpha'_+)}_{\tau'}(\vec{r}')\right]|HFB\rangle \\ &\eta^{-1}_{k\tau,k'\tau'} = \eta^{-1}_{k'\tau',k\tau} \equiv \mathrm{i}\langle HFB|\left[\hat{Q}_{k'\tau'},\hat{P}_{k\tau}\right]|HFB\rangle = \\ &= \int \mathrm{d}^3 r \int \mathrm{d}^3 r' \sum_{\alpha_-\alpha'_-} \langle HFB|\left[\hat{Q}_{k\tau},\hat{J}^{(\alpha_-)}_\tau(\vec{r})\right]|HFB\rangle \left[\frac{\partial^2\mathcal{E}}{\partial J^{(\alpha_-)}_\tau(\vec{r})\partial J^{(\alpha'_-)}_{\tau'}(\vec{r}')}\right] \\ &\quad \langle HFB|\left[\hat{Q}_{k'\tau'},\hat{J}^{(\alpha'_-)}_{\tau'}(\vec{r}')\right]|HFB\rangle \end{aligned} \tag{2.26}$$

For the determination of the vibration amplitudes $\overline{q}_{k\tau}$ and $\overline{p}_{k\tau}$ (see (2.19)) and corresponding vibration frequencies ω we use time-dependent-Hartree-Fock-Bogoliubov (TDHFB) method starting from the Thouless theorem for

the vibrating $|HFB(t)\rangle$ vacuum:

$$|HFB(t)\rangle_\nu = \mathrm{e}^{\sum\limits_{\overline{\omega}=ij,\overline{ij},i\overline{j}} c_{\overline{\omega}}^{(\nu)}(t) b_{\overline{\omega}}^\dagger} |HFB\rangle \approx \left(1 + \sum_{\overline{\omega}=ij,\overline{ij},i\overline{j}} c_{\overline{\omega}}^{(\nu)}(t) b_{\overline{\omega}}^\dagger\right) |HFB\rangle \tag{2.27}$$

where

$$c_{\overline{\omega}}^{(\nu)} = c_{\overline{\omega}}^{(\nu)+} \mathrm{e}^{\mathrm{i}\omega_\nu t} + c_{\overline{\omega}}^{(\nu)} \mathrm{e}^{-\mathrm{i}\omega_\nu t}$$

and where $b_{ij}^\dagger$, $b_{\overline{ij}}^\dagger$, $b_{i\overline{j}}^\dagger$ are two-quasiparticle quasi-boson operators

$$b_{ij}^\dagger = \alpha_i^\dagger \alpha_j^\dagger \qquad\qquad b_{\overline{ij}}^\dagger = \alpha_{\overline{i}}^\dagger \alpha_{\overline{j}}^\dagger \qquad\qquad b_{i\overline{j}}^\dagger = \alpha_i \alpha_{\overline{j}}^\dagger \tag{2.28}$$

with

$$\begin{aligned}
\langle HFB| \left[b_{ij}, b_{i'j'}^\dagger\right] |HFB\rangle &= \delta_{ii'}\delta_{jj'} - \delta_{ij'}\delta_{ji'} \\
\langle HFB| \left[b_{\overline{ij}}, b_{\overline{i'j'}}^\dagger\right] |HFB\rangle &= \delta_{ii'}\delta_{jj'} - \delta_{ij'}\delta_{ji'} \\
\langle HFB| \left[b_{i\overline{j}}, b_{i'\overline{j'}}^\dagger\right] |HFB\rangle &= \delta_{ii'}\delta_{jj'}
\end{aligned} \tag{2.29}$$

Using TDHFB equation

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} |HFB(t)\rangle_\nu = \left[\hat{h}_{HFB} + \delta\hat{h}_{HFB}(t)\right] |HFB(t)\rangle_\nu \tag{2.30}$$

we express amplitudes $c_{\overline{\omega}}^{\pm}$ in terms of $\overline{q}_{k\tau}$ and $\overline{p}_{k\tau}$ and then, substituting into (2.27) we determine ${}_\nu\langle HFB|\delta\hat{X}_{k\tau}|HFB\rangle_\nu$ and $\langle HFB|\delta\hat{Y}_{k\tau}|HFB\rangle$. By comparison of these expectation values with the previous ones (see (2.25)) we finally obtain the system of equations for unknown amplitudes $\overline{q}_{k\tau}$, $\overline{p}_{k\tau}$:

$$\begin{aligned}
\sum_{\tau' k'} \Big[\quad \overline{q}_{k'\tau'}^{(\nu)} \left[F_{k'\tau',k\tau}^{(XX)} - \kappa_{k'\tau',k\tau}^{-1}\right] + \qquad\qquad \overline{p}_{k'\tau'}^{(\nu)} F_{k'\tau',k\tau}^{(XY)} \Big] &= 0 \\
\sum_{\tau' k'} \Big[\qquad\qquad \overline{q}_{k'\tau'}^{(\nu)} F_{k'\tau',k\tau}^{(YX)} + \quad \overline{p}_{k'\tau'}^{(\nu)} \left[F_{k'\tau',k\tau}^{(YY)} - \eta_{k'\tau',k\tau}^{-1}\right] \Big] &= 0
\end{aligned} \tag{2.31}$$

where we introduced following matrices

$$\begin{aligned}
F_{k\tau,k'\tau'}^{(AA)}(\hbar\omega) &= \sum_{\overline{\tau}} \sum_{\substack{\overline{\omega}\in\overline{\tau} \\ \overline{\omega}=ij,i\overline{j},\overline{ij}}} \frac{\varepsilon_{\overline{\omega}} \langle\overline{\omega}|\hat{A}_{k'\tau'}^{\overline{\tau}}|\rangle \langle\overline{\omega}|\hat{A}_{k\tau}^{\overline{\tau}}|\rangle}{\varepsilon_{\overline{\omega}}^2 - \hbar^2\omega^2} \\
F_{k'\tau',k\tau}^{(AB)}(\hbar\omega) &= F_{k\tau,k'\tau'}^{(BA)}(\hbar\omega) = \sum_{\overline{\tau}=n,p} \sum_{\substack{\overline{\omega}\in\overline{\tau} \\ \overline{\omega}=ij,i\overline{j},\overline{ij}}} \frac{\hbar\omega \langle\overline{\omega}|\hat{A}_{k'\tau'}^{\overline{\tau}}|\rangle \langle\overline{\omega}|\hat{A}_{k\tau}^{\overline{\tau}}|\rangle}{\varepsilon_{\overline{\omega}}^2 - \hbar^2\omega^2}
\end{aligned} \tag{2.32}$$

where $\hat{A}$, $\hat{B} = \hat{X}_{k\tau}$ or $\hat{Y}_{k\tau}$. In (2.32) $\langle\overline{\omega}|\hat{A}_{k\tau}|\rangle$ ($\overline{\omega} = ij, i\overline{j}, \overline{ij}$) are two-quasiparticle matrix elements of given operator $\hat{A}$, and $\varepsilon_{\overline{\omega}}$ are two-quasiparticle energies:

$$\varepsilon_{\overline{\omega}} = \begin{cases} E_i + E_j & \text{for } \overline{\omega} = ij \\ E_i + E_{\overline{j}} & \text{for } \overline{\omega} = i\overline{j} \\ E_{\overline{i}} + E_{\overline{j}} & \text{for } \overline{\omega} = \overline{ij} \end{cases} \tag{2.33}$$

It should be noted that the matrix of the eq. system (2.31) is hermitian (real and symmetric). The dimension of the equation system (2.31) is $4N$ where N is the number of excited nucleus $(\hat{Q}_k, \hat{P}_k)$ $(k = 1, \ldots, N)$ - see (2.17). The index ν in (2.31) enumerates all solutions of the eq. system (2.31). The condition of solvability of the eq. system (2.31) is that the determinant of its matrix is zero

$$\det F(\omega_\nu) = 0 \tag{2.34}$$

where F is the matrix of the system (2.31). Equation (2.34) gives energies $\hbar\omega_\nu$ of all TDHFB solutions.
It can be shown that the equation system (2.31) for unknown $\overline{q}^{(\nu)}_{k\tau}$ and $\overline{p}^{(\nu)}_{k\tau}$ is the same as the one obtained from the standard static RPA equations

$$\left[\hat{H}_{RPA}, \hat{O}^\dagger_\nu\right] = \hbar\omega_\nu \hat{O}^\dagger_\nu \qquad \left[\hat{H}_{RPA}, \hat{O}_\nu\right] = -\hbar\omega_\nu \hat{O}_\nu$$
$$\left[\hat{O}_\nu, \hat{O}^\dagger_{\nu'}\right] = \delta_{\nu\nu'} \tag{2.35}$$

if we take the RPA Hamiltonian in the form

$$\hat{H}_{RPA} = \hat{h}_{HFB} + \hat{V}^{(SRPA)}_{res} \tag{2.36}$$

where $\hat{h}_{HFB}$ is the HFB mean field (2.13) and $\hat{V}^{(SRPA)}_{res}$ is the separable residual RPA interaction

$$\hat{V}^{(SRPA)}_{res} = \sum_{k\tau} \sum_{\substack{k'\tau' \\ k,k'=1,\ldots,N}} \left\{ \kappa_{k\tau,k'\tau'} \hat{X}^{(1)}_{k\tau} \hat{X}^{(1)}_{k'\tau'} + \eta_{k\tau,k'\tau'} \hat{Y}^{(1)}_{k\tau} \hat{Y}^{(1)}_{k'\tau'} \right\} \tag{2.37}$$

where $\hat{X}^{(1)}_{k\tau}$, $\hat{Y}^{(1)}_{k\tau}$ is a two-quasiparticle part of the corresponding operators $\hat{X}_{k\tau}$ and $\hat{Y}_{k\tau}$ (parts involving only $\alpha^\dagger\alpha^\dagger$ and $\alpha\alpha$ terms in their quasiparticle representation expressions). The symbols $\hat{O}^\dagger_\nu$, $\hat{O}_\nu$ in (2.35) stand for the creation and annihilation operator of oscillation quanta (in the nuclear physics they are called phonons) with the corresponding RPA vacuum $|RPA\rangle$:

$$\hat{O}_\nu |RPA\rangle = 0 \tag{2.38}$$

for all RPA or TDHFB solutions ν. In the framework of the RPA, phonon operators $\hat{O}^{\dagger}_{\nu}$ have two-quasiparticle character:

$$\hat{O}^{\dagger}_{\nu} = \sum_{\tau=n,p} \sum_{\substack{\overline{\omega}\in\tau \\ \overline{\omega}=ij,\overline{ij},i\overline{j}}} \left\{ \psi^{(\nu,\tau)}_{\overline{\omega}} b^{\dagger}_{\overline{\omega}} - \varphi^{(\nu,\tau)}_{\overline{\omega}} b_{\overline{\omega}} \right\} \tag{2.39}$$

and two-quasiparticle amplitudes $\psi^{(\nu,\tau)}_{\overline{\omega}}$ and $\varphi^{(\nu,\tau)}_{\overline{\omega}}$ are related to the solutions $\overline{q}_{k\tau}$ and $\overline{p}_{k\tau}$ of the TDHFB equation system (2.31) by following relations:

$$\begin{aligned} \psi^{(\nu,\tau)}_{\overline{\omega}} &= 4\xi_{\overline{\omega}} \frac{\sum\limits_{\tau' k'} \overline{q}^{(\nu)}_{k'\tau'} \langle \overline{\omega} | \hat{X}^{\tau}_{k'\tau'} | \rangle - \mathrm{i} \sum\limits_{\tau' k'} \overline{p}^{(\nu)}_{k'\tau'} \langle \overline{\omega} | \hat{Y}^{\tau}_{k'\tau'} | \rangle}{\varepsilon_{\overline{\omega}} - \hbar\omega_{\nu}} \\ \varphi^{(\nu,\tau)}_{\overline{\omega}} &= 4\xi_{\overline{\omega}} \frac{\sum\limits_{\tau' k'} \overline{q}^{(\nu)}_{k'\tau'} \langle \overline{\omega} | \hat{X}^{\tau}_{k'\tau'} | \rangle + \mathrm{i} \sum\limits_{\tau' k'} \overline{p}^{(\nu)}_{k'\tau'} \langle \overline{\omega} | \hat{Y}^{\tau}_{k'\tau'} | \rangle}{\varepsilon_{\overline{\omega}} + \hbar\omega} \end{aligned} \tag{2.40}$$

where

$$\xi_{\overline{\omega}} = \begin{cases} \frac{1}{4} & \text{for } \overline{\omega} = ij \\ \frac{1}{4} & \text{for } \overline{\omega} = \overline{ij} \\ \frac{1}{2} & \text{for } \overline{\omega} = i\overline{j} \end{cases} \tag{2.41}$$

So, practical recipe for the description of nuclear excitations in the framework of our HFB + SRPA approach is following

- At first we solve the HF variational problem (2.10) self-consistently with BCS problem (2.12) – (2.16). As a result we obtain HF single-particle basis (i.e. single-particle states $|i\rangle = a^{\dagger}_{i}|\rangle$ with corresponding single-particle energies e_i) with the corresponding occupation quasiparticle amplitudes $\mathcal{U}_i$ and $\mathcal{V}_i$ and quasiparticle energies E_i (see (2.16))

- In the next step we choose the exciting modes ($\hat{Q}_k$, $\hat{P}_k$)$(k = 1, \ldots, N)$ adequately to the type and multipolarity of the investigated excitations.

- Then we construct the matrix F of the RPA system of equations (2.31) and by solving this equation system we obtain unknowns $\overline{q}^{k\tau}_{(\nu)}$, $\overline{p}^{k\tau}_{(\nu)}$ with corresponding phonon energies $\hbar\omega_{\nu}$. The structure, that means amplitudes $\psi^{(\nu,\tau)}_{\overline{\omega}}$ and $\varphi^{(\nu,\tau)}_{\overline{\omega}}$ (see (2.39)), of each one-phonon state $|\nu\rangle \equiv \hat{O}^{\dagger}_{\nu}|RPA\rangle$ is then given by (2.40).

Knowing the structure and energy spectrum of nucleus excitation $|\nu\rangle = \hat{O}^{\dagger}_{\nu}|RPA\rangle$ we can determine reduced transition probabilities of the transitions from the RPA ground state $|RPA\rangle$ into the one-phonon excited state $|\nu\rangle$ with the energy $\hbar\omega_{\nu}$ (see e.g. [3]):

$$\begin{aligned} B(Z\lambda\mu;\,|RPA\rangle \to |\nu\rangle) &= \left|\langle RPA|[\hat{O}^{\dagger}_{\nu}, \hat{M}^{(1)}_{Z\lambda\mu}]|RPA\rangle\right|^2 = \\ &= \left|\sum_{k\tau}\left\{\overline{q}^{(\nu)}_{k\tau} A^{(X)(Z\lambda\mu)}_{k\tau;\omega_{\nu}} + \overline{p}^{(\nu)}_{k\tau} A^{(Y)(Z\lambda\mu)}_{k\tau;\omega_{\nu}}\right\}\right|^2 \end{aligned} \tag{2.42}$$

where $\hat{M}^{(1)}_{Z\lambda\mu}$ is the two-quasiparticle part of the transition operator responsible for given transition of type Z (Z = electric or Z = magnetic) with the multipolarity λ with the projection μ. In (2.42) we introduced the following symbols:

$$\begin{aligned} A^{(X)(Z\lambda\mu)}_{k\tau;\omega_{\nu}} &\equiv 2\sum_{\tau'=n,p}\sum_{\substack{\overline{\omega}\in\tau' \\ \overline{\omega}=i\overline{j},\overline{i}j,i\overline{j}}} \frac{g_1\langle\overline{\omega}|\hat{X}^{\tau'}_{k\tau}|\rangle\langle\overline{\omega}|\hat{M}_{Z\lambda\mu}|\rangle}{\varepsilon^2_{\overline{\omega}} - \hbar^2\omega^2_{\nu}} \\ A^{(Y)(Z\lambda\mu)}_{k\tau;\omega_{\nu}} &\equiv 2\sum_{\tau'=n,p}\sum_{\substack{\overline{\omega}\in\tau' \\ \overline{\omega}=i\overline{j},\overline{i}j,i\overline{j}}} \frac{g_2\langle\overline{\omega}|\hat{Y}^{\tau'}_{k\tau}|\rangle\langle\overline{\omega}|\hat{M}_{Z\lambda\mu}|\rangle}{\varepsilon^2_{\overline{\omega}} - \hbar^2\omega^2_{\nu}} \end{aligned} \tag{2.43}$$

where $g_1 = \varepsilon_{\overline{\omega}}$, $g_2 = \hbar\omega_{\nu}$ for an electric type (Z = el.) transition and $g_1 = \hbar\omega_{\nu}$, $g_2 = \varepsilon_{\overline{\omega}}$ for a magnetic type (Z = mag.) transition. Reduced transition probabilities (2.42) can be also rewritten as following

$$B(Z\lambda\mu;\,|RPA\rangle \to |\nu\rangle) = \left[\sum_{k\tau}\sum_{k'\tau'} A^{\dagger}_{k\tau}(\omega_{\nu}) F_{k\tau,k'\tau'} A_{k'\tau'}(\omega_{\nu})\right]\left[\frac{\partial}{\partial\omega}\det F\right]^{-1}_{\omega=\omega_{\nu}} \tag{2.44}$$

where

$$\begin{aligned} A_{k\tau}(\omega) &\equiv \begin{pmatrix} A^{(X)(Z\lambda\mu)}_{k\tau;\omega} \\ \\ A^{(Y)(Z\lambda\mu)}_{k\tau;\omega} \end{pmatrix} \\ F_{k\tau,k'\tau'} &\equiv \begin{pmatrix} F^{(XX)}_{k\tau,k'\tau'} & F^{(XX)}_{k\tau,k'\tau'} \\ \\ F^{(YX)}_{k\tau,k'\tau'} & F^{(XX)}_{k\tau,k'\tau'} \end{pmatrix} \end{aligned} \tag{2.45}$$

If we know all RPA solutions $|\nu\rangle$ and corresponding excitation probability $B(Z\lambda\mu;\,|RPA\rangle \to |\nu\rangle)$ then we can determine the energy weighted strength function $S_L(Z\lambda\mu; E)$ defined as

$$S_L(Z\lambda\mu; E) = \sum_{\nu} B(Z\lambda\mu;\,|RPA\rangle \to |\nu\rangle)(\hbar\omega_\nu)^L \delta(E - \hbar\omega_\nu) \tag{2.46}$$

This quantity represents the energy weighted distribution of the reduced excitation probability of the transitions of type Z with the multipolarity λ with the projection μ. It is possible to determine this strength function (2.46) without explicitly solving the RPA equation (see e.g. [3]). This possibility is based on replacing Dirac function $\delta(E - \hbar\omega_\nu)$ in (2.46) by the Lorentzian averaging function:

$$\begin{aligned} \xi_\Delta(E - \hbar\omega_\nu) &= \frac{1}{2\pi} \frac{\Delta}{(E - \hbar\omega_\nu) + \left(\frac{\Delta}{2}\right)^2} \\ \lim_{\Delta\to 0} \xi_\Delta(E - \hbar\omega_\nu) &= \delta(E - \hbar\omega_\nu) \end{aligned} \tag{2.47}$$

then after the substitution for $B(Z\lambda\mu;\,|RPA\rangle \to |\nu\rangle)$ (see (2.44)) in (2.46) and using Cauchy theorem (see [3]) we obtain the final expression

$$\begin{aligned} S_L(Z\lambda\mu; E) = \mathrm{Im} \left[\frac{z^L \sum_{k\tau} \sum_{k'\tau'} A^\dagger_{k\tau}(z) F_{k\tau,k'\tau'}(z) A_{k'\tau'}(z)}{\pi \det F(z)} \right]_{z=E+\mathrm{i}\frac{\Delta}{2}} + \\ + \frac{\Delta}{\pi} \sum_{\substack{\overline{\omega} \\ \overline{\omega}=i\overline{j},\overline{ij},i\overline{j}}} \varepsilon^L_{\overline{\omega}} \left| \langle\overline{\omega}|\hat{M}_{Z\lambda\mu}|\rangle \right|^2 \left\{ \frac{1}{(E - \varepsilon_{\overline{\omega}})^2 + \left(\frac{\Delta}{2}\right)^2} - \frac{1}{(E + \varepsilon_{\overline{\omega}})^2 + \left(\frac{\Delta}{2}\right)^2} \right\} \end{aligned} \tag{2.48}$$

where the first term is a contribution coming from the residual interaction and the second term is the contribution from the mean field.

3 Discussion of results

3.1 Description of numerical codes

The chain of numerical codes (in FORTRAN) was developed in collaboration of the University in Erlangen, the JINR Dubna in Russia and the Institute of Particle and Nuclear Physics of Charles University. These codes firstly solve the selfconsistent HFB problem, to determine the mean-field and the corresponding one-(quasi)particle spectrum. Then follows the solution of the separable RPA - we gain the energies $\hbar\omega_\nu$, and structure (that means amplitudes $\psi^\nu_{\overline{\omega}}$, $\phi^\nu_{\overline{\omega}}$, $\overline{\omega} = ij, i\overline{j}, \overline{i}\overline{j}$ - see (2.39)) of RPA phonons $|\nu\rangle = \hat{O}^\dagger_\nu|RPA\rangle$. These codes also calculate reduced probabilities $B(Z\lambda\mu, |RPA\rangle \rightarrow |\nu\rangle)$ of excitation transitions of electric (Z = el.) and magnetic (Z = mag.) type with different multipolarities λ of projection μ. We gain also corresponding energy weighted distributions of these reduced probabilities (strength functions $S_L(Z\lambda\mu; E)$). Codes are based on the HFB + SRPA approach with Skyrme functionals described in the previous chapter.
The chain of codes consists of three codes: `SKYAX.f`, `SKYAX_me.f`, `SKYAX_srpa.f`. Below we characterize briefly each of these programs.

`SKYAX` – This program calculates the HFB ground state using the HFB variational method. In the input file we specify the even-even nucleus which is the object of our calculation and also parametrization of the Skyrme functional for the constrained HFB equations.

`SKYAX_me` – This program calculates one-particle (or one-quasiparticle) matrix elements of given operators $\hat{Q}_k$, $\hat{P}_k$ ($k = 1, \ldots, N$) (these we determine in the input file) for a specific type and multipolarity of $Z\lambda\mu$ transitions and transition operators $M_{Z\lambda\mu}$. It also determines matrix elements of the operators $\hat{X}_k$ and $\hat{Y}_k$ in RPA residual interaction (see (2.23),(2.24)).

`SKYAX_srpa` – This program reads matrix elements from the previous program and constructs separable RPA matrix (see (2.32)), then it solves the separable RPA equation (2.31) and calculates energies and a structure of the phonons $|\nu\rangle$ excited by a given set of operators ($\hat{Q}_k$, $\hat{P}_k$). It also determines given strength function $S_L(Z\lambda\mu; E)$.

3.2 Isovector electric dipole and isoscalar electric quadrupole giant resonances in ^{92,102}Mo

Codes described above were used for analysis of the electric giant dipole resonance (GDR) and the electric giant quadrupole resonance (GQR) in two nuclei, ^{92}Mo and ^{102}Mo. These resonances were calculated using four different Skyrme interaction parametrizations: `SkM*, SkT6, SLy6, SkI3`. These parametrizations were chosen because they cover a wide interval of the nuclear effective masses ($m^*/m \in (0.58 - 1.0)$) (see e.g. [5]). The nuclei were chosen, because isotope ^{92}Mo is spherical while ^{102}Mo is deformed, as it can be seen from the figs. (Fig. 3.1) and (Fig. 3.2). So by the comparison of results for ^{92}Mo with those for ^{102}Mo we can analyze the effect of a deformation.

Here it is worth to explain what we mean by the words "shape of nucleus" in more detail. From the point of view of microscopic models, nothing as the sharp edge of nucleus does exist. However, in the models based on the density functional techniques (e.g. Skyrme Hartree-Fock) as well as in the Shell Model, we can introduce the equipotential surfaces of the static mean-field. It is possible to express any general (unambiguous) surface using the Dirichlet's decomposition

$$R(\theta,\varphi) = R_0(1 + \sum_{l=1}^{\infty}\sum_{m=-l}^{+l} \alpha_{lm} Y_{lm}(\theta,\varphi)), \tag{3.1}$$

where $R(\theta,\varphi)$ is the distance between the origin of the coordinate system (nucleus center of mass) and the point on the mean field equipotential surface, in the direction given by the angles θ, φ in the spherical coordinate system. In (3.1) $Y_{lm}(\theta,\varphi)$ are the spherical functions, R_0 is the mean radius, and α_{lm} are the deformation parameters. In this work we focus only on the nuclei deformed axially which means: $\alpha_{20} \equiv \beta \neq 0$ and all other α_{lm} ($\lambda \geq 0$) are zero [1]. In the case of spherical nuclei we have $\alpha_{lm} = 0$ for all l, m.

The cranked HFB variational problem - used in the code `SKYAX` for the determination of the deformation parameter β - is nothing more than the method of the Lagrange multipliers where we fix the mean value of the quadrupole operator with the projection $\mu = 0$ ($\langle HFB|\hat{M}_{20}|HFB\rangle$) to the

[1] It is possible to prove that all α_{1m} values are zero since they are related to the translations of nucleus as a whole. The parameter α_{00} specifies the compressibility of the nucleus but since it is possible to include it in the value of the mean radius R_0, we do not discuss this point in more detail.

value corresponding to the deformation β - for more detailed study of this point see e.g. [8]. In practice we run the cranked HFB calculation on a grid of β-parameter values in the interval $\beta \in \langle \beta_{min}, \beta_{max} \rangle$ and find the minimum of the total energy $E_{tot} = \langle HFB|\hat{H}|HFB\rangle$. In this way we find an equilibrium deformation β.

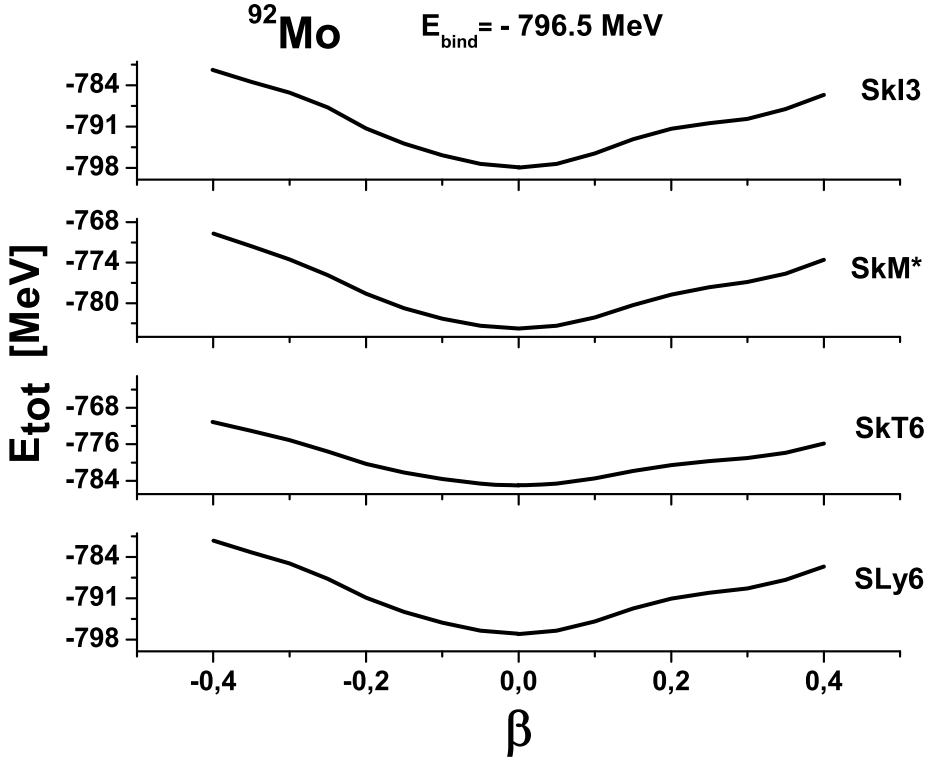

Figure 3.1: Dependence of the total nucleus energy $E_{tot} = \langle HFB|\hat{H}|HFB\rangle$ on a quadrupole deformation parameter β in ^{92}Mo for different Skyrme interaction parametrizations.

In the figs. (Fig. 3.1) and (Fig. 3.2) we plot the dependences of the total energy E_{tot} on the constraint value of the deformation parameter β for ^{92}Mo and ^{102}Mo, respectively. From these figures it is seen that ^{92}Mo is spherical (equilibrium value of β is zero) for all investigated parametrizations. In the case of ^{102}Mo, can be distinguished two minima for each parametrization. Minimum of E_{tot} in the interval $\beta \sim 0.38 - 0.43$ corresponds to the prolate ellipsoidal shape, whereas the negative minimum with $\beta \sim -0.22$

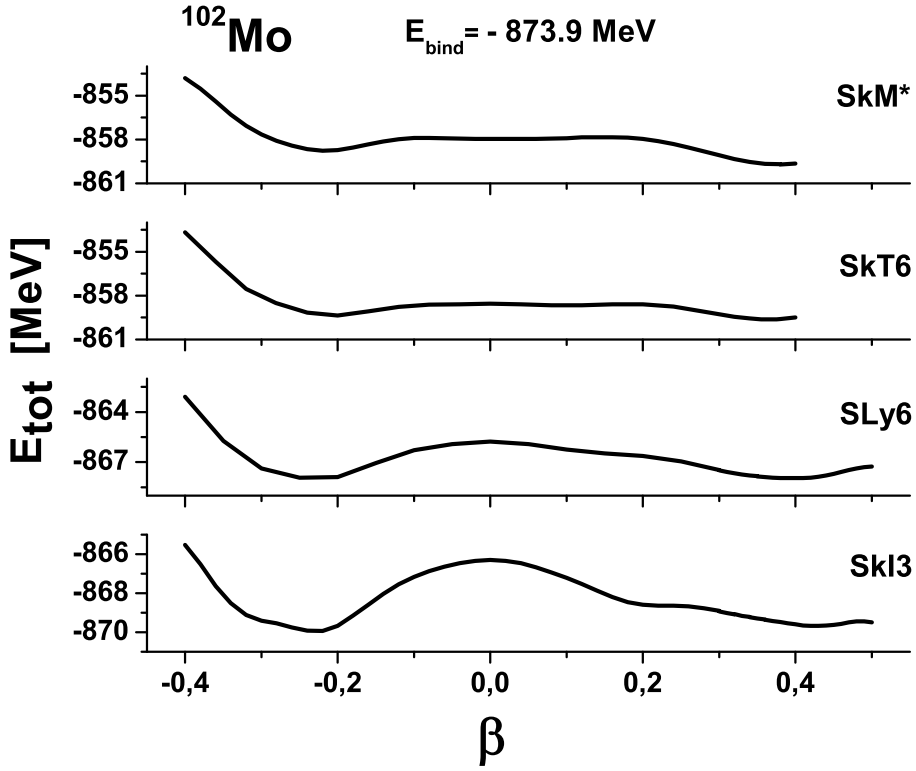

Figure 3.2: Dependence of the total nucleus energy $E_{tot} = \langle HFB|\hat{H}|HFB\rangle$ on a quadrupole deformation parameter β in ^{102}Mo for different Skyrme interaction parametrizations.

is characteristic for oblate ellipsoidal shape. It should be noted that several experimental facts measured for ^{102}Mo are more likely in agreement with the prolate minimum. In Figs. 1 and 2 are also noted (just for comparison) the experimental values of the total binding energies E_{bind} of the nuclei obtained experimentally from measurements of the mass of the nuclei. It can be seen that the different parametrizations predict different values of the total energy E_{tot}. This is possible to explain by the fact that Skyrme parametrizations are usually fitted to the nuclear properties of several nuclei - usually doubly magic. Evidently the qualities of several Skyrme parametrizations start to differ while we study "less common" nuclei (nuclei with neutron excess, far from the line of stability). In case of the nuclei we study in this work (^{92}Mo, ^{102}Mo), the `SkI3` parametrization is the most close to the experimental values of the binding energies E_{bind}.

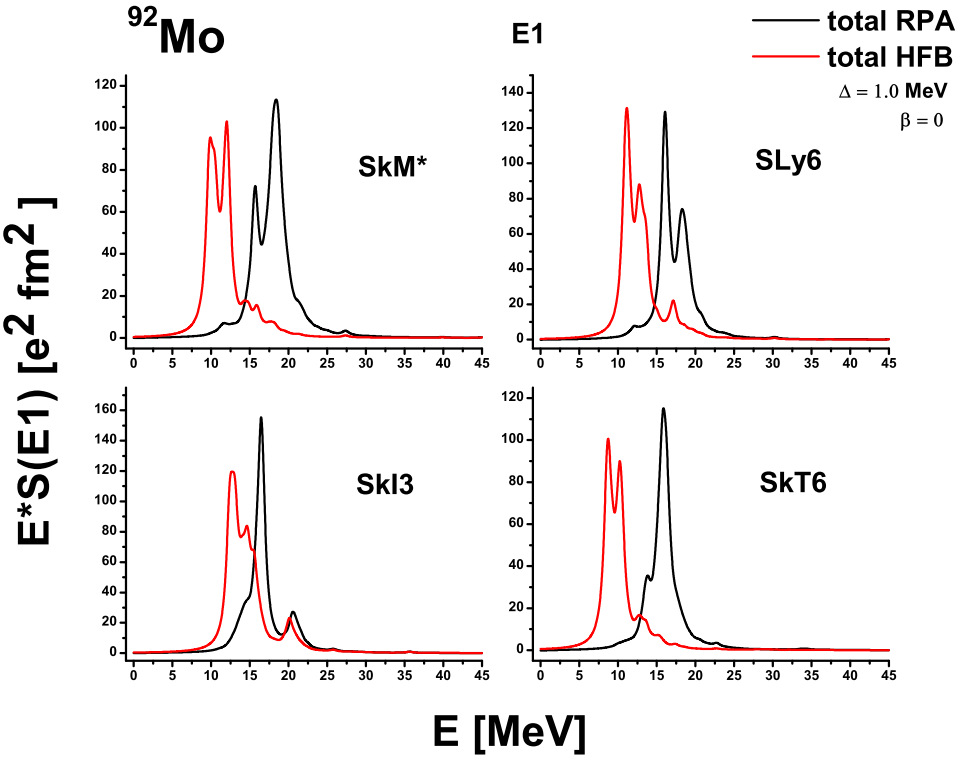

Figure 3.3: Dependence of the energy weighted strength function $S(E1;E)$ for ^{92}Mo for different Skyrme interaction parametrizations calculated both by including and not including a residual interaction.

In the figs. (Fig. 3.3) and (Fig. 3.4) we show the energy weighted strength functions $S_1(E1;E) = \sum_{\mu=0,1} S_1(E1\mu;E)$ for ^{92}Mo and ^{102}Mo, calculated according to the formula (2.48) for different Skyrme interaction parametrizations. Similarly in the figs. (Fig. 3.5) and (Fig. 3.6) are shown the energy weighted strength functions for quadrupole excitations, $S_1(E2;E)$.

In all these figures we compare perturbed (that include the residual interaction using the separable RPA method) and unperturbed (static mean field calculation) strength functions.

As we might see in the figures (Fig. 3.4) and (Fig. 3.5), when we switch on the residual interaction, peaks of the giant resonance shift to the higher energies for isovector E1 transitions, or to the lower energies for isoscalar E2 transitions. Peak of the quadrupole giant resonances is wider than in the E1 case. This phenomenon occurs due to the Landau fragmentation ef-

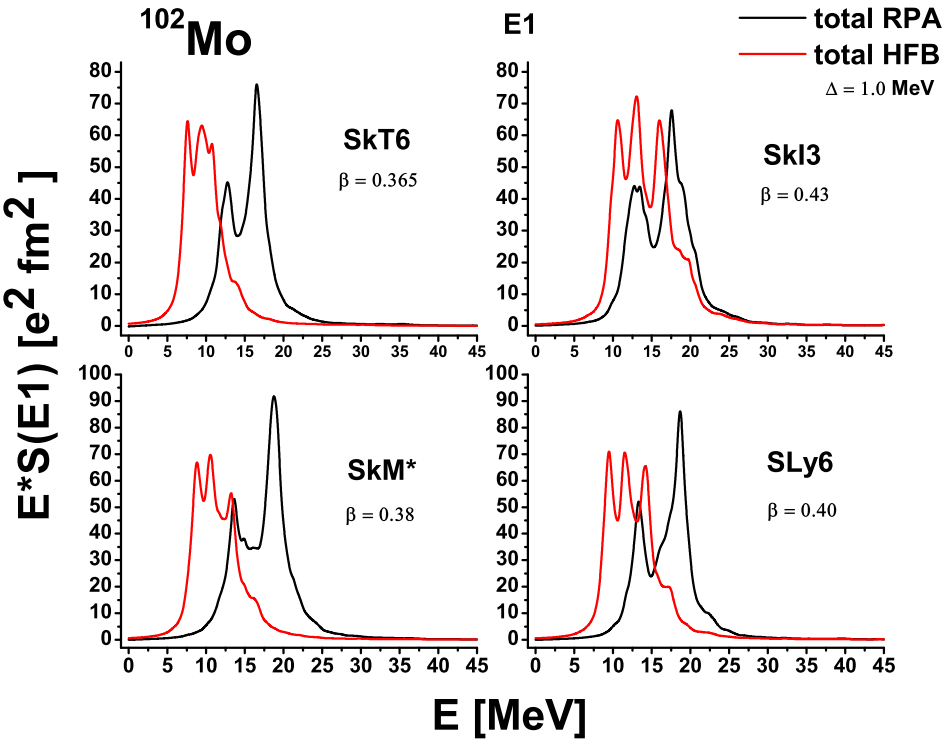

Figure 3.4: Dependence of the energy weighted strength function $S(E1;E)$ for ^{102}Mo for different Skyrme interaction parametrizations calculated both by including and not including a residual interaction.

fect (a distribution of the collective strength between close two-quasiparticle states). These two-quasiparticle configurations are more dense in the case of E2 excitations which leads to the stronger contribution of the Landau fragmentation into the total width of an E2 giant resonance peak (in comparison with the E1) - see e.g. [2].

Similarly, by comparing the spherical nucleus ^{92}Mo with the axially deformed ^{102}Mo, we might see the giant resonance peak (in both cases in E1 as well as E2) is more wide in the deformed case. This effect takes part due to the deformation splitting. In the deformed case the giant resonance exhibits different energy shifts for all projections μ whereas in the spheric nuclei the strength from all projections sums into one peak. This is also verified in the figs. (Fig. 3.7) and (Fig. 3.8) where are plotted the strength functions for all projections μ as well as the total strength function.

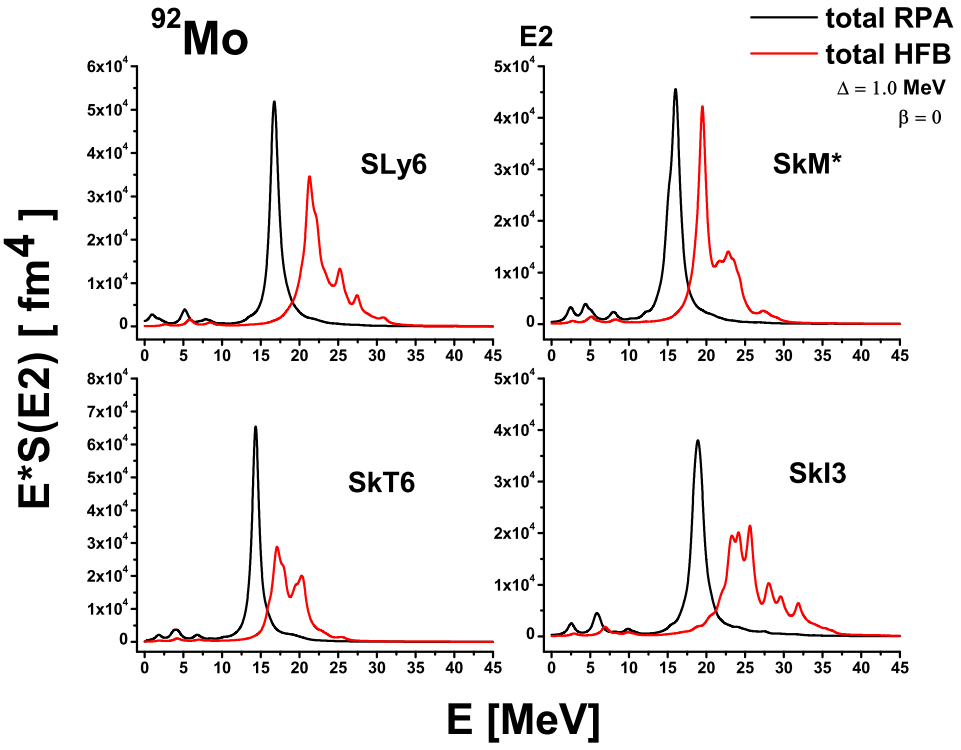

Figure 3.5: Dependence of the energy weighted strength function $S(E2;E)$ for ^{92}Mo for different Skyrme interaction parametrizations calculated both by including and not including residual interaction.

In the figs. (Fig. 3.7) and (Fig. 3.8) are plotted the total strength functions calculated by SRPA method together with the strength functions for the individual projections μ. On the graphs for ^{92}Mo we might see that the strength functions for all projections of the angular momentum are degenerated in their shapes (the amplitude for the $\mu = 1$ projection is twice as big as that for $\mu = 0$ which is caused by the fact that we sum the projections $\mu = +1$ and $\mu = -1$ into one curve). Analogically we sum the projections $\mu = +2$ with $\mu = -2$ and $\mu = +1$ with $\mu = -1$ in the case of the E2 resonance. Even in the case of the deformed nucleus ^{102}Mo - where the peaks of strength functions are of different energies for the different projections μ - their maxima are approximately in ratio 1:2 for $\mu = 0/\mu = 1$ and 1:2:2 for $\mu = 0/\mu = 1/\mu = 2$.
In the Figs. 3.7 and 3.8 we add, for comparison, the empiric values for the po-

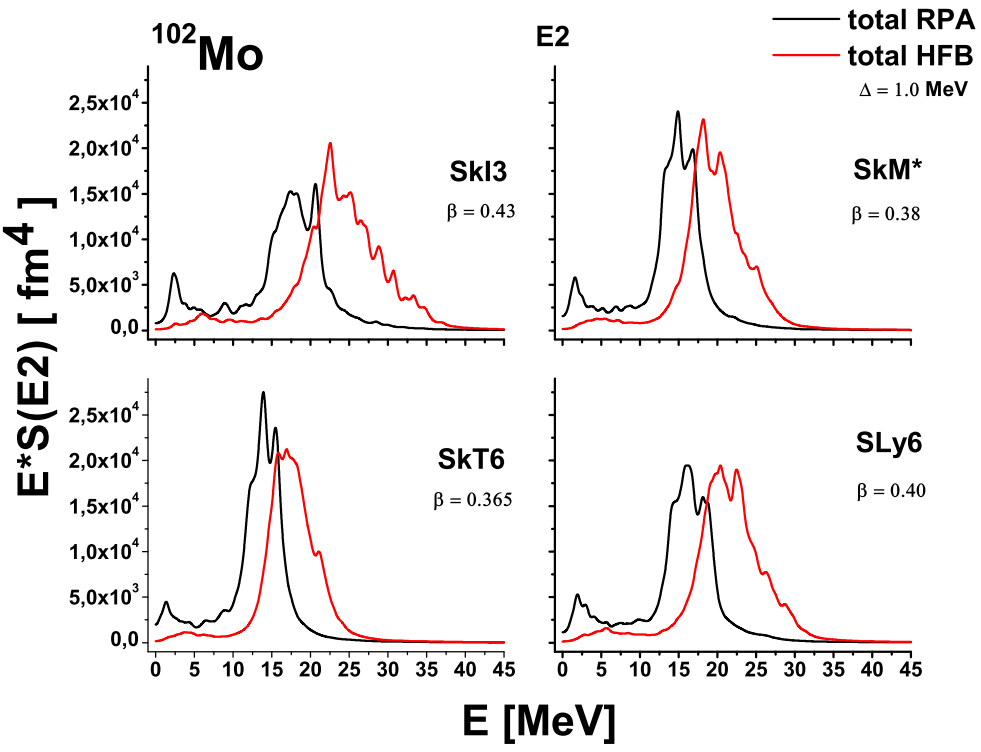

Figure 3.6: Dependence of the energy weighted strength function $S(E2;E)$ for ^{102}Mo for different Skyrme interaction parametrizations calculated both by including and not including residual interaction.

sition of the isovector E1 giant resonance $E \approx (31.2A^{-1/3} + 20.6A^{-1/6})$MeV and the isoscalar E2 giant resonance $E \approx 65A^{-1/4}$MeV - see the textbook [1].

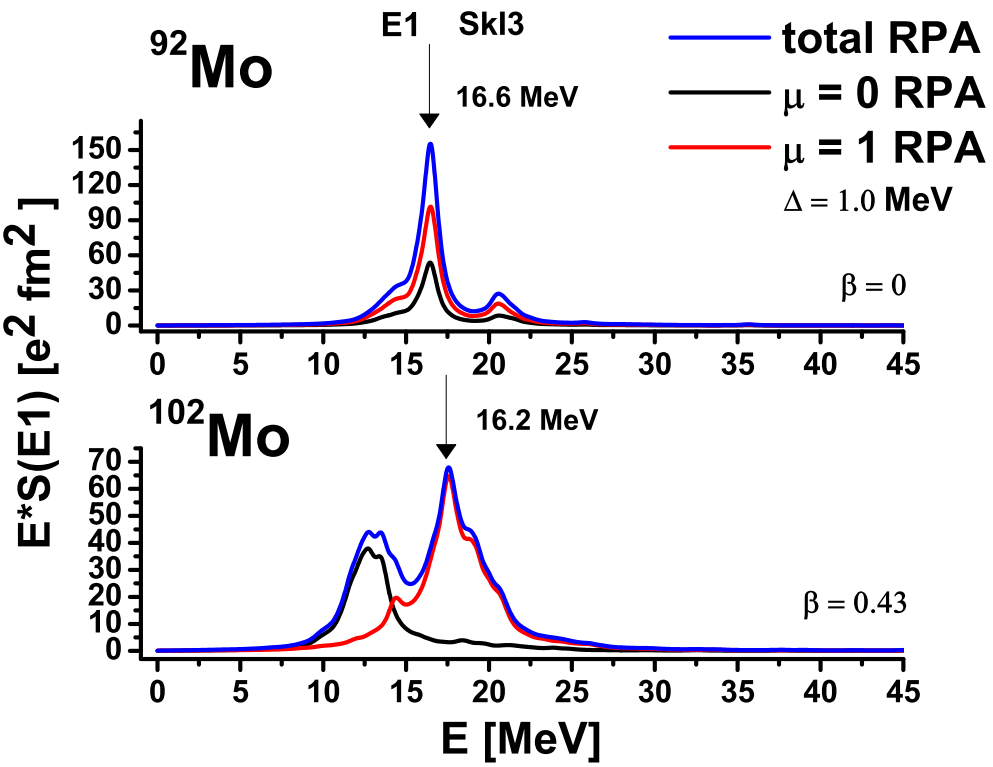

Figure 3.7: Energy weighted strength functions $S(E1;E)$ for $\mu = 0, 1$ and total strength function, for SkI3 Skyrme interaction parametrization.

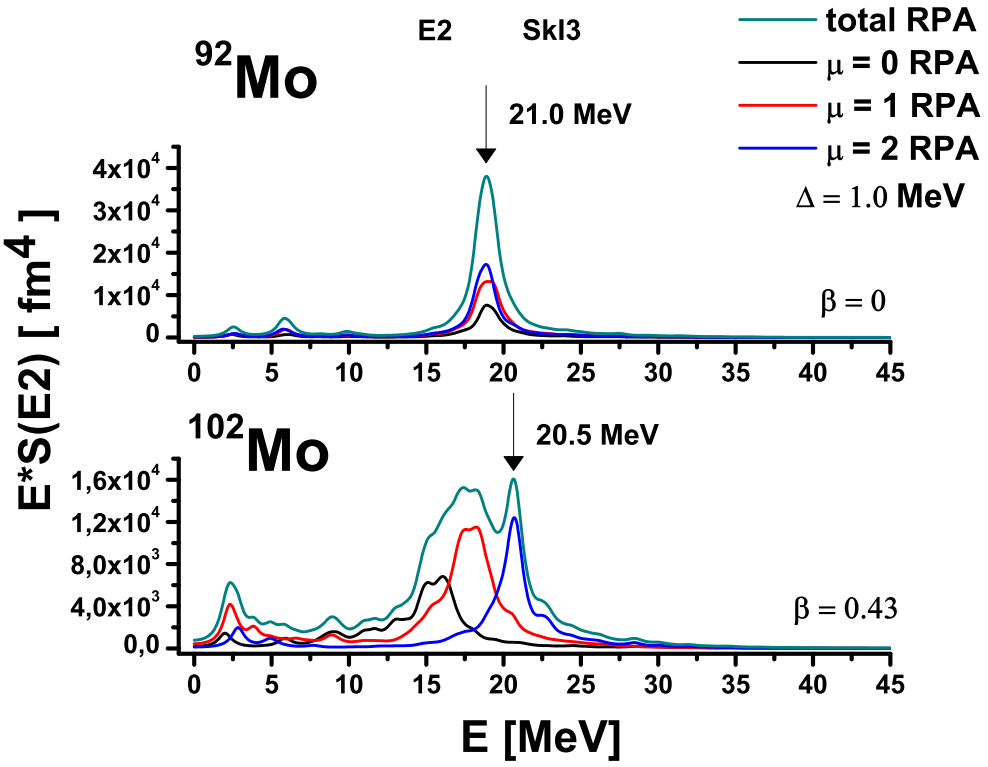

Figure 3.8: Energy weighted strength functions $S(E2;E)$ for $\mu = 0, 1, 2$ and total strength function, for SkI3 Skyrme interaction parametrization.

4 Conclusion

In this bachelor thesis I got acquainted with the Hartre-Fock-Bogoliubov + separable Random-Phase-Approximation method. HFB allows us to selfconsistently construct the nuclear mean-field. Separable RPA is going beyond the static mean-field approach and takes into account also a residual interaction. Within this model we calculated the strength functions for the electromagnetic transitions in heavier nuclei. Four different parametrisations of the effective Skyrme interaction were used.

The method is implemented into the chain of codes `SKYAX.f`, `SKYAX_me.f` and `SKYAX_srpa.f`. The goal of our calculations was to compare the strength functions of isovector E1 and isoscalar E2 transitions in ^{92}Mo and ^{102}Mo. The ^{92}Mo isotope was chosen as an example of a spherical nucleus, the nucleus ^{102}Mo as an example of the axially deformed nucleus. In the case of a deformed nucleus we observe the giant resonance splitting due to different shifts of the resonance for different projections μ, whereas for the spherical nucleus all projections sum up into one peak.

We also observed the energy shift of the giant resonances caused by the residual interaction. In the case of the isovector E1 transition the giant resonance is shifted up in comparison with the (static) mean-field approach. On the contrary in the isoscalar E2 case we observe shift down in the energy.

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